Letters to the Editor

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THE CRYSTAL STRUCTURE OF BENZALAZINE

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In an earlier communication (Sinha, 1959), the space group of benzalazine along with other crystallograhic data has already been published. However, the axial lengths were redetermined from high angle Bragg reflections in Weissenberg photographs by the method of Lipson and Farquhar (1946), after necessary correction for film-shrinkage error, etc. The revised values of the axial parameters thus obtained are

$$\left.\begin{aligned} a_0 &= 13.09\ \text{Å} \\ b_0 &= 11.76\ \text{Å} \\ c_0 &= 7.62\ \text{Å} \end{aligned}\right\} \quad \alpha = \beta = \gamma = 90^\circ,$$

the space-group being D^{12}_{2h}—Pbcn, containing four molecules per unit cell. This space-group containing a centre of symmetry has eight equivalent points in the unit cell. The structural formula of the molecule of benzalazine is C_6H_5 . CH : N. N : CH. C_6H_5. It shows that the molecule has a centre of symmetry. This indicates that the centre of the N—N bond must lie at the centre of symmetry which has been chosen to be the origin of the coordinates.

The relative intensities of the reflections *hko*, *hol* and *okl* were measured by photographic method, absolute values were obtained by comparing these with the known absolute values of F_{hkl} of aluminium and hence the structure factors were obtained.

The intensity of (002) diffuse reflection suggested that the orientation of the benzene ring of the molecule would be near about (001) plane. In addition, by a consideration of the high intensity (*hko*) reflections of higher indices using the method adopted by Robertson and White (1945) for coronane, the approximate co-ordinates (x, y) were obtained after giving a few trials. Using these trial coordinates, the phases of the structure factors were calculated for computing the electron density projection $\rho(x\,y\,o)$ along [001] with the observed values of the structure factors F(*hko*). The preliminary structure thus obtained was refined by three successive [001] axis Fourier projections to give the more and more accurate values of x and y co-ordinates. Trial z-coordinates were worked out from the standard bond lengths of the molecule in order to calculate the phases of (*hol*) reflections. The z-coordinates were finally determined from the second electron density projection $\rho(xoz)$ obtained with the observed values of F(*hol*). The co-ordinates of the benzalazine molecule are given in Table I.

TABLE I

Atoms	X in Å	Y in Å	Z in Å
N	0.69_1	0.12_7	$+0.07$
C_1	1.23_9	1.00_3	-0.32_0
C_2	2.68_3	1.26_8	0.16_5
C_3	3.27_2	2.40_6	-0.66
C_4	4.60_3	2.66_5	0.50_8
C_5	5.40	1.76_4	$+0.14_6$
C_6	4.84_3	0.62_7	$+0.63_5$
C_7	3.49_5	0.36_2	$+0.49$

The reliability index factor

$$R = \frac{\Sigma|(|F_o| - |F_c|)|}{\Sigma|F_o|}$$

came out to be 0.20 for F(*hko*) reflections and 0.24 for F(*hol*) reflections. In the calculation of the structure factors, the atomic scattering factors for carbon and nitrogen (McWeeny, 1951) have been used after imposing an isotropic B-factor of 3.00×10^{-16}.

The structure of benzalazine is being further refined by the method of difference synthesis and other standard methods and the detailed results will be published in near future.

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